Line-Edge Blending in ATOMIC

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Aline-edge blending algorithm was introduced into ATOMIC to eliminate an erroneous gap in absorption spectra and to provide a smooth transition into higher density where continuum lowering and the disappearance of spectral lines occur. The erroneous absorption gap occurs in the region where the calculated atomic physics data ends for a Rydberg series of photo-excitations, usually determined by a principal quantum number cut-off, and where the photo-ionization edge begins at the binding energy of the ionizing electron. Line-edge blending can have a significant effect on the calculated opacity.

The first step to accomplish this scheme is to extend the bound-free cross section to photon energies below the photo-ionization edge. Software was developed to identify the Rydberg series of spectral lines leading up to each edge. Then using the Rydberg series oscillator strengths, a table of extended cross sections is built internally with photon energies corresponding to the particular final n state leading up to that edge. Thus, the entire procedure is automated. For the present time only edges with initial states of $n \leq 3$ are considered.

For a given density and temperature, the EOS computation provides occupation probabilities, ϕ for every level that is included in the calculation. The occupation probability is the probability that a particular state has not disappeared due to density effects. Therefore the intensity of spectral lines must be decreased by the factor ϕ and the corresponding extrapolated bound-free cross section is multiplied with the factor $(1-\phi)$ in order to conserve total oscillator strength.

At low densities the occupation probabilities are near unity. As density increases, the values for ϕ decrease with the most highly excited levels decreasing the fastest.

An interpolation table is constructed to calculate the bound-free cross section for each density, temperature, and edge combination. It consists of the photo-ionization cross section for energies at and above the edge and the bound-free extension scaled by $(1-\phi)$ for energies below the tabulated limit, usually n = 10. An additional point is included at 25% of the distance between the tabulated series energy limit and the ionization edge to ensure the gap fills in smoothly.

Figure 1 illustrates line-edge blending computed by ATOMIC for different plasma ion densities for the Lyman Rydberg series of hydrogen-like oxygen. The electron temperature is held fixed at 60 eV for each calculation. The curve labeled NB corresponds to the calculation at an ion density of 10^{18} ions per cubic centimeter without line-edge blending. The gap in the calculation from the last n = 10 line in the data (863 eV) to the photo-ionization edge (872 eV) is evident. Note that the gap is filled in for the calculation at the same density including line-edge blending. Also note that as the ion density is increased the lines become broader with decreased magnitude. At an ion density of 10^{20} spectral lines below n = 10 start to disappear and by a density of 10^{22} the entire series from n = 3 to n = 10 has sunk into the continuum.

***For more information, contact
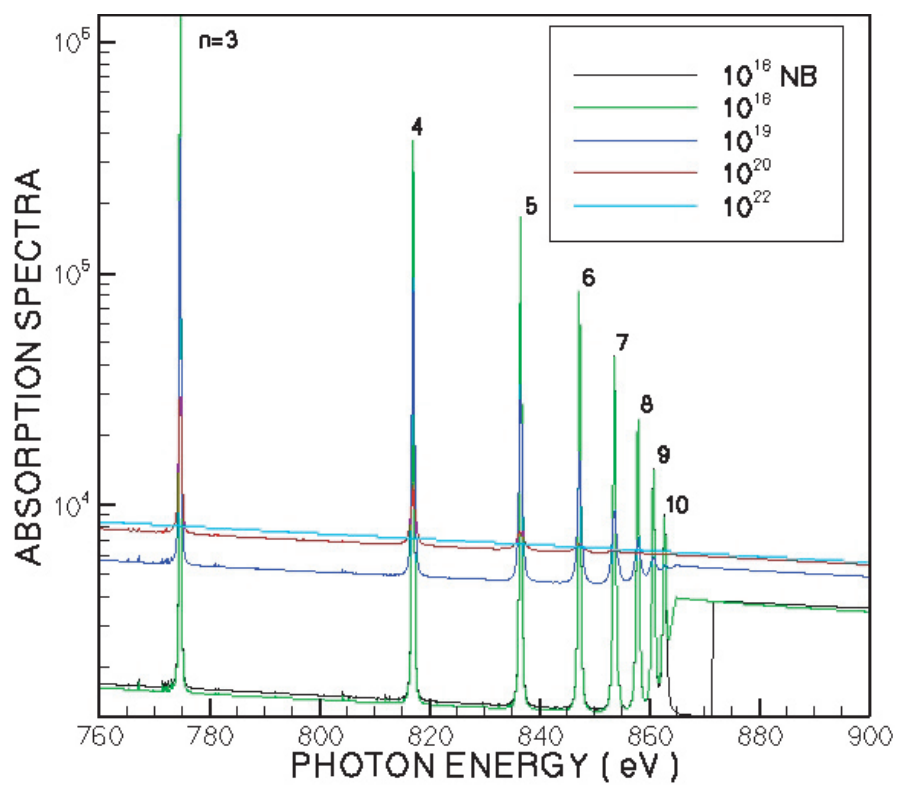Joseph Abdallah (abd@lanl.gov).***

Figure 1—
Line-edge blending
computed by ATOMIC
for different plasma
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hydrogen-like oxygen.